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A New Procedure for Integrating the Point Kinetic Equations for Fission Reactors

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Abstract—This work deals with a new technique for the numerical integration of the system of differential equations that constitutes the so-called "*point reactor kinetics model*" in the physics of fission reactors. The technique is based on an exact analytic integration of the reactor power equation, associated to an iterative procedure, that allows the estimate of the best parabolic interpolation of the precursor concentrations, consistently with the requirement of making the whole set of differential equations simultaneously satisfied.

This very unusual approach can allow time steps as large as several tens of seconds, provided that the reactivity curve, inside each one of them, can be best fitted linearly to an acceptable accuracy. This technique could be used not only in real time power reactor forecasting, in order to prevent reactivity accidents, but also for carrying out highly accurate calculations of the space dependent power transients, whenever a space eigenfunctions expansion of the neutron distribution can be easily performed. This could provide benchmark references to some finite difference or finite elements numerical codes to be adopted in reactor safety assessments.

Keywords—Reactor kinetics, Differential equations, Numerical integration.

1. INTRODUCTION AND PHYSICAL BACKGROUND

This paper is concerned with a new method for the quick integration of the system of ordinary differential equations usually referred to as the "*point reactor kinetics*" model in nuclear reactor dynamics. These equations are usually met when, starting from very detailed transport [1] or multigroup diffusion [2] models of fission reactor kinetics, one attempts to set up the simplest dynamical procedure for analyzing and controlling the energy released by a fission power plant. Despite the crude approximation embodied into the point reactor kinetic equations and the recently improved techniques for solving the space and time dependent problems, this model can still be expected to play a very important role in the future. As far as it can be used, when properly solved, for an almost real time forecasting of the reactor power transients, it will

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allow timely control intervention on the plant, in order to prevent the raising of severe accident conditions [3,4].

A well-known difficulty of this integration comes from the stiff character of the equations themselves [5,6]. (See also the references in Y. Ronen [7].) Associated to the need of getting almost real time answers, if the target of a safer nuclear era is to be achieved.

In order to clarify all the essential mathematical features of the new approach presented in this research, still preventing from the need of too cumbersome a notation, we shall refer here to *the simplest physical model* of the problem at hand. This involves as unknown functions only the time dependent total reactor power $P(t)$ and the total content $C(t)$ of precursors of delayed fission neutrons. All of the precursors are thus assumed to constitute a unique radioactive family, with its own average decay constant $\lambda\,[\mathrm{sec}^{-1}]$. Furthermore, a unique value of the overall yield β of delayed neutron precursors per fission neutron produced is required by the model. The constant $l\,[\mathrm{sec}]$, the prompt neutron lifetime, is a key physical parameter of theory.

In this paper, instead of the standard problem, involving, together with the power output $P(t)$, the $R > 1$ concentrations $C_i(t)$ of precursor families, that takes, in presence of an external neutron source $S(t)$, the classical form [2]

$$\begin{aligned} \frac{dP(t)}{dt} &= \frac{\rho(t)-\beta}{l}P(t) + \sum_{i=1}^{R}\lambda_i C_i(t) + S(t), \\ \frac{dC_i(t)}{dt} &= \frac{\beta_i}{l}P(t) - \lambda_i C_i(t), \qquad i = 1,2,\dots R, \end{aligned} \tag{1}$$

where, usually, $R = 6$, $\beta \doteq \sum_{i=1}^{R}\beta_i$, and $\rho(t)$, the so-called *reactivity function*, is a known input variable in linear dynamics, to be supplemented by the following set of initial conditions:

$$P(t=0) = P_0, \qquad C_i(t=0) = C_{i0}, \qquad i = 1,2,\dots R, \tag{1'}$$

we will consider only its much simpler form, leading to the system

$$\begin{aligned} \frac{dP(t)}{dt} &= \frac{\rho(t)-\beta}{l}P(t) + \lambda C(t), \\ \frac{dC(t)}{dt} &= \frac{\beta}{l}P(t) - \lambda C(t) \end{aligned} \tag{2}$$

with

$$\begin{aligned} P(0) &= P_0, \\ C(0) &= C_0, \end{aligned} \tag{2'}$$

subjected to the further restriction of absence of any external sources.

In this model, the only two constant initial values required, i.e., $P(0) = P_0$ and $C(0) = C_0$, are usually known in one of the following ways:

(i) if the reactor operation was *stationary up to the time* $t = 0$, the conventional instant at which the "reactivity" $\rho(t)$ starts to become different from zero, then the value P_0 is assigned by the condition $P_0 = P(t<0) = \text{const}$, while the ratio P_0/C_0 *must* assume its equilibrium value, consistent with the stationary solution of equation (2), i.e., the unique value

$$\frac{P_0}{C_0} = \frac{\lambda l}{\beta}. \tag{3}$$

If the above starting condition is not realized, any arbitrary couple of real and positive initial values, for both P_0 and C_0, can be accepted.

(ii) if we assume, as it is the case in the present work, that the time axis can be partitioned, for computational convenience, in a set of contiguous time intervals $I_k \doteq [t_k,\ t_{k+1} > t_k]$,

of length $\Delta t_k \doteq (t_{k+1} - t_k)$, within each one of them the *"reactivity" function $\rho(t)$ has a linear time behaviour*[1], then, during the calculation of a particularly long lasting (i.e., involving several I_k) transient, when we are inside a given time interval $[t_k, t_{k+1}]$ $(k > 1)$, the initial values to be used for both P and C are those calculated at the right end of the previous interval.

The essential feature of the "hybrid" integration method that we propose consists of subjecting to completely different mathematical treatments the two unknown functions P and C, on the basis of the following physical information. The power function $P(t)$ can be expected to undergo extremely rapid transients under a set of so called "accident," but otherwise physically conceivable, conditions. On the contrary, the total content of precursors $C(t)$ happens to be, as a rule, a slowly varying function of time, even when we were faced with an explosive reactor behavior. This is a consequence of the fact that the overall precursor content in a reactor results from a cumulative effect, related to the previous power history as a whole.

So even a tremendous power excursion happens to have, at least in its initial phase, a rather limited and, so to say, a quite delayed effect in sharpening the rise of $C(t)$.

These facts are well-known to nuclear reactor physicists; see, for instance, [7]. Their knowledge has been exploited in the past, whenever approximate, and still uncomputerized procedures for integrating the point kinetic equations have been set up.

In this work, we shall assume at first that, within a given I_k, in which the rate of growth of reactivity takes a constant value, the function $C(t)$ can be suitably interpolated by *a second degree polynomial of* $(t - t_k)$, with unknown coefficients.

Furthermore, an iterative algorithm is developed that allows us to determine the best estimate of these coefficients, along with the fulfillment of the whole set of differential equations (2).

This fulfillment is accomplished, to be specific, in a very particular, although physically adequate, subspace of the unknown "state vectors"

$$|X(t)\rangle \doteq \left|\begin{matrix} P(t) \\ C(t) \end{matrix}\right\rangle. \tag{2''}$$

For that subspace, the second component of $|X(t)\rangle$ is restricted to be a second order polynomial, while its first component $P(t)$ is, at last, determined *analytically*, through an "hybrid" technique. This is involving a progressive adjustment of the parabola's coefficients, based on a practically unlimited set of successive iterations, with each step being made, so to say, for improving the consistency of the iterated precursor concentrations with the power evolution equation. The goal of establishing the limit power behavior is achieved through a highly efficient numerical calculation of a few integrals, easily derived from the equations by means of fully analytical integration processes. As we shall see presently, this technique makes mathematically selfconsistent the procedure of calculating the coefficients of the "best parabolic representation" of $C(t)$, together with that of making both equations (2) satisfied.

Let us, first of all, set up the following nomenclature, concerning the k^{th} time interval I_k and any given *continuous* functions $g(t)$:

$$g(t) \doteq g_k(t), \qquad \forall t \in]t_k, t_{k+1}[; \tag{4}$$

$$g_k(t_k) \doteq g_k^-, \qquad g_k(t_{k+1}) \doteq g_k^+ \equiv g_{k+1}^-, \qquad k \in \mathbb{N}. \tag{4'}$$

[1]This problem, often referred to as that of the "reactivity ramp insertion," has been solved exactly in the fifties by means of a very complicated, but fully analytical procedure. That result could constitute, of course, a benchmark reference for all the approximate techniques, although it is rather unpractical, by its own nature, as a real time power forecasting tool. See, for details, [1, Chapter 3].

Furthermore, to be specific, for $t \in I_k$, we assume

$$\begin{aligned} \rho(t) \doteq \rho_k(t) &= \rho(t_k) + \alpha_k(t - t_k) \\ &= \rho_k^- - \alpha_k t_k + \alpha_k t \\ &\doteq \rho_k^* + \alpha_k t. \end{aligned} \tag{5}$$

The α_k's have been taken as real, positive, or at least nonnegative, constants in the present treatment. This choice covers the more interesting safety problems. And also

$$\rho(t_{k+1}) = \rho_k^+ = \rho_{k+1}^-.$$

The last equality applies unless a reactivity jump, to be specified as a result of either a sudden action of some control device or, a conventional, stepwise insertion of feedback contributions, is allowed at the right boundary of the k^{th} time interval.

Each constant α_k, the so-called reactivity insertion rate, is, in principle, different from the ones related to both the previous and successive interval.[2]

After defining

$$\beta_k \doteq \beta - \rho_k^* \tag{6}$$

inside the k^{th} time interval our problem can thus be written

$$\begin{aligned} \frac{dP_k}{dt} &= \frac{\alpha_k t - \beta_k}{l} P_k + \lambda C_k, \\ \frac{dC_k}{dt} &= \frac{\beta}{l} P_k - \lambda C_k \end{aligned} \tag{7}$$

associated to the initial condition

$$P(t_k) \doteq P_k^- = \begin{cases} P_{k-1}^+, & \text{previously calculated, or, for } k = 1, \text{ either} \\ P_0 \equiv P(t < 0), & \text{or } P_0 \text{ arbitrary,} \end{cases}$$

and

$$C(t_k) \doteq C_k^- = \begin{cases} C_{k-1}^+, & \text{previously calculated, or, for } k = 1, \text{ either} \\ C_0 = \dfrac{P_0 \beta}{\lambda l}, & \text{or } C_0 \text{ arbitrary,} \end{cases} \tag{8}$$

as the case may be.

2. THE HYBRID ITERATIVE PROCEDURE

Let us define

$$\gamma_k(t) \doteq \frac{\alpha_k t - \beta_k}{l} \tag{9}$$

and

$$\Gamma_k(t) \doteq \frac{\alpha_k}{2l}\left(t^2 - t_k^2\right) - \frac{\beta_k}{l}(t - t_k). \tag{10}$$

For the above functions, the following relationships hold:

$$\Gamma_k(t_k) = 0, \qquad \frac{d\Gamma_k}{dt} = \gamma_k, \qquad \Gamma_k(t) = \int_{t_k}^{t} \gamma_k(t')dt'. \tag{11}$$

[2]The only exceptions to the above statement could come into play quite artificially, when the convergence of the integration process is not achieved over the whole extent of a given I_k. In such a case, as we will show presently, I_k needs to be fractioned, for purely computational reasons, thus creating two or more further subintervals, out of the main one I_k. Let us call them $I_{k_1}, I_{k_2}, \ldots$. Obviously for all of them the same α_k applies. The values of $\rho_{k_1}^*, \rho_{k_2}^*, \ldots$ and those of the corresponding $\beta_{k_1}, \beta_{k_2}, \ldots$, however, as a consequence of the definitions (5) and (6), will come out to be different from one another.

At this stage we notice that a "formal" time integration inside each one of the equations of the differential system (7), account being taken of the initial condition (8), leads to the system of nonhomogeneous Volterra integral equations

$$P_k(t) = e^{\Gamma_k(t)} \left[P_k^- + \lambda \int_{t_k}^{t} C_k(t') e^{-\Gamma_k(t')}\, dt' \right], \tag{12a}$$

$$C_k(t) = C_k^- e^{-\lambda(t-t_k)} + \frac{\beta}{l} \int_{t_k}^{t} P_k(t') e^{-\lambda(t-t')}\, dt', \qquad t \in I_k. \tag{12b}$$

Before presenting our integration procedure, let us define *an iteration index* (j), to be written as a top right label, after each function.

Assume furthermore that, within I_k, as the zeroth iteration for the function $C_k(t)$ one can take, as a rule, a constant value, according to

$$C_k^{(0)}(t) = C_k^- = \text{const}, \qquad \forall t \in I_k, \quad \forall k \tag{13}$$

and then define the j^{th} iteration for the power according to

$$P_k^{(j)}(t) \stackrel{\text{def}}{=} e^{\Gamma_k(t)} \left[P_k^- + \lambda \int_{t_k}^{t} \tilde{C}_k^{(j-1)}(t') e^{-\Gamma_k(t')}\, dt' \right], \tag{14}$$

together with the j^{th} iteration for the $C_k(t)$ in the form

$$\tilde{C}_k^{(j)}(t) \stackrel{\text{def}}{=} C_k^- e^{-\lambda(t-t_k)} + \frac{\beta}{l} \int_{t_k}^{t} P_k^{(j)}(t') e^{-\lambda(t-t')}\, dt'. \tag{15}$$

Notice that, conventionally, the iteration index j increases by one when passing from the right side to the left one in equation (14), that defines the next estimate of the power in terms of the previous precursors' knowledge. On the contrary, the iteration index is left unchanged in (15), thus establishing that the j^{th} estimate of $\tilde{C}_k(t)$ is consistent with the j^{th} estimate of the power. In equations (14), (15) and (18) the physical unknown $C_k(t)$ has been reported as the oversigned function $\tilde{C}(t)$. This is due to the opportunity of assigning the name $C(t)$ to the parabolic interpolation of the actual precursor concentration (see equation (19) below) and not to the concentration itself.

To be specific, in order to clarify the algorithm we refer, from here on, to the first time interval, starting from an equilibrium reactor situation for $t < 0$, although we still keep the index k as if it were unspecified. Thus, $P_k^- = P\ (t < 0)$; $C_k^- = P_k^-(\beta/\lambda l) \doteq C_k^{(0)}(t)$. Let us then write down explicitly, in this particular case, the first iteration for the power

$$P_k^{(1)}(t) = \frac{\beta}{l} P_k^- e^{\Gamma_k(t)} \left\{ \int_{t_k}^{t} e^{-\Gamma_k(t')}\, dt' + \frac{l}{\beta} \right\} \tag{16}$$

or, once the integration has been carried out,

$$P_k^{(1)}(t) = \frac{\beta}{l} P_k^- e^{(\alpha_k t + \beta_k)^2} \left[\frac{\sqrt{\pi}}{2\alpha_k} (\operatorname{erf}(\alpha_k t + \beta_k) - \operatorname{erf}(\alpha_k t_k + \beta_k)) + \frac{l}{\beta} e^{-\beta_k^2} e^{-\left((\alpha_k t_k^2/2l) - \beta_k (t_k/l)\right)} \right]. \tag{17}$$

As far as the first iteration for the precursors content is concerned, we establish to evaluate it according to (15)

$$\tilde{C}_k^{(1)}(t) = C_k^- e^{-\lambda(t-t_k)} + \frac{\beta}{l} \int_{t_k}^{t} P_k^{(1)}(t') e^{-\lambda(t-t')}\, dt'. \tag{18}$$

We can anticipate at this stage that the explicit evaluation of the last integral, the integrand function being taken from (17), is about to lead to a great amount of computational difficulties.

A deeper investigation about these difficulties, which turn out to be somehow related to stiff character of the differential system (2), will be presented later on. Let us assume for the moment that, irrespective of the technique being used, an accurate estimate of the right-hand side of (18) can be provided.

Unfortunately, however, the next step, for passing analytically from $\tilde{C}_k^{(1)}(t)$ to $P_k^{(2)}(t)$ according to equation (14) would become definitely unpractical. Obviously the situation would still worsen for the successive steps, where the difficulties streaming from the algorithm sum up to those related to the stiffness. Actually this amounts to making unquestionably useless the iterative procedure (14) and (15), no matter how trivial the choice of the zeroth step for $C(t)$ has been.

At this stage the following parabolic representation for $\tilde{C}_k^{(j)}(t)$ is adopted:

$$C_k^{(j)}(t) = C_k^- + c_{k,1}^{(j)}(t - t_k) + c_{k,2}^{(j)}(t - t_k)^2, \tag{19}$$

where, in agreement with a previous choice, $a_{k,1}^{(0)} = a_{k,2}^{(0)} = 0$.

The unknown coefficients $c_{k,1}^{(j)}$ and $c_{k,2}^{(j)}$, *starting from* $j = 1$, are determined through the conditions that the representation (19) must coincide with $\tilde{C}_k^{(j)}(t)$, as expressed by (18), at the instants $t = (t_k + (\Delta t_k)/2)$ and $t = (t_k + \Delta t_k) \doteq t_{k+1}$, the agreement at t_k being already assured by the structure of the formulas being adopted.

This amounts to the fulfillment of the following linear nonhomogeneous system for the unknowns $c_{k,l}^{(j)}$'s:

$$\begin{aligned} c_{k,1}^{(j)}\Delta t_k + c_{k,2}^{(j)}\frac{(\Delta t_k)^2}{2} &= 2\left[\tilde{C}_k^{(j)}\left(t_k + \frac{\Delta t_k}{2}\right) - C_k^-\right] \doteq b_{k,1}^{(j)}, \\ c_{k,1}^{(j)}\Delta t_k + c_{k,2}^{(j)}(\Delta t_k)^2 &= \left[\tilde{C}_k^{(j)}(t_{k+1}) - C_k^-\right] \doteq b_{k,2}^{(j)}. \end{aligned} \tag{20}$$

These *linearly independent equations* can be easily solved, with the following results:

$$c_{k,1}^{(j)} = \frac{2b_{k,1}^{(j)} - b_{k,2}^{(j)}}{\Delta t_k}, \tag{21a}$$

$$c_{k,2}^{(j)} = \frac{2\left(b_{k,2}^{(j)} - b_{k,1}^{(j)}\right)}{(\Delta t_k)^2}. \tag{21b}$$

The known parameters $b_{k,i}^{(j)}$'s have been defined through the rightmost statements of equation (20) themselves. So the explicit representation of $C_k^{(j)}(t)$ comes out in the form

$$C_k^{(j)}(t) = C_k^- + \frac{2b_{k,1}^{(j)} - b_{k,2}^{(j)}}{\Delta t_k}(t - t_k) + \frac{2\left(b_{k,2}^{(j)} - b_{k,1}^{(j)}\right)}{(\Delta t_k)^2}(t - t_k)^2. \tag{22}$$

Let us go back now to (14), in which the previous change $j \to (j+1)$ has been made and $\tilde{C}_k$ has been replaced by C_k, $\forall j$, and $\forall t \in I_k$. According to (19),

$$\begin{aligned} P_k^{(j+1)}(t) &= e^{\Gamma_k(t)}\left[P_k^- + \lambda\int_{t_k}^t C_k^{(j)}(t')e^{-\Gamma_k(t')}\,dt'\right] \\ &= e^{\Gamma_k(t)}\left[P_k^- + \lambda\int_{t_k}^t \left[C_k^- + c_{k,1}^{(j)}(t' - t_k) + c_{k,2}^{(j)}(t' - t_k)^2\right]e^{-\Gamma_k(t')}\,dt'\right] \end{aligned} \tag{23}$$

or, in more compact, writing, after particularizing at first equation (16) for $j = 1$

$$P_k^{(j+1)}(t) = P_k^{(1)}(t) + e^{\Gamma_k(t)}\lambda\sum_{m=1}^{2} c_{k,m}^{(j)}\int_{t_k}^t (t' - t_k)^m e^{-\Gamma_k(t')}\,dt', \tag{24}$$

that can be presented in its final form

$$P_k^{(j+1)}(t) = P_k^{(1)}(t) + \lambda \sum_{m=1}^{2} c_{k,m}^{(j)} T_{k,m}(t), \tag{25}$$

as soon as the following definitions:

$$T_{k,m}(t) = e^{\Gamma_k(t)} \int_{t_k}^{t} (t' - t_k)^m e^{-\Gamma_k(t')}\, dt', \qquad m = 1, 2 \tag{26}$$

have been introduced. A very important property of the functions $T_{k,m}$'s is their independence of the iteration index j.

A further progress toward establishing our algorithm is achieved when one introduces (25) into (15), rewritten after the change $j \to (j+1)$. This will allow us to calculate the two constants

$$\tilde{C}_k^{(j+1)}\left(t_k + \frac{\Delta t_k}{2}\right) \doteq C_k^{*(j+1)}; \quad \tilde{C}_k^{(j+1)}(t_{k+1}) \doteq C_k^{**(j+1)}, \tag{26'}$$

through two particular evaluations of

$$\begin{aligned} \tilde{C}_k^{(j+1)}(t) = C_k^- e^{-\lambda(t-t_k)} &+ \frac{\beta}{l} \int_{t_k}^{t} P_k^{(1)}(t') e^{-\lambda(t-t')}\, dt' \\ &+ \frac{\beta\lambda}{l} \sum_{m=1}^{2} c_{k,m}^{(j)} \int_{t_k}^{t} T_{k,m}(t') e^{-\lambda(t-t')}\, dt'. \end{aligned} \tag{27}$$

This formula can be given a still more compact form after writing

$$\tilde{C}_k^{(j+1)}(t) = C_k^- e^{-\lambda(t-t_k)} + \frac{\beta}{l}\Theta_{k,0}(t) + \frac{\beta\lambda}{l} \sum_{m=1}^{2} c_{k,m}^{(j)} \Theta_{k,m}(t), \tag{27'}$$

where the following definitions have be introduced:

$$\begin{aligned} \Theta_{k,0}(t) &= \int_{t_k}^{t} P_k^{(1)}(t') e^{-\lambda(t-t')}\, dt', \\ \Theta_{k,m}(t) &= \int_{t_k}^{t} T_{k,m}(t') e^{-\lambda(t-t')}\, dt', \qquad m = 1, 2. \end{aligned} \tag{28}$$

To represent the particular values of the three functions Θ's just defined both at the middle and rightmost point of I_k, we use the following six starred symbols:

$$\begin{aligned} \Theta_{k,m}^{*} &\doteq \Theta_{k,m}\left(t_k + \frac{\Delta t_k}{2}\right), \\ \Theta_{k,m}^{*} + \Theta_{k,m}^{**} &\doteq \Theta_{k,m}(t_{k+1}), \qquad m = 0, 1, 2. \end{aligned} \tag{29}$$

The twice starred variables play obviously the role of integrals, extended over the subinterval $[t_k + (\Delta t_k)/2,\ t_{k+1}]$, $\forall k$. Thus, a twofold evaluation of (27'), account being taken of (26'), (28) and (29), leads to the couple of equations

$$\begin{aligned} C_k^{*(j+1)} &= C_k^- e^{-\lambda(\Delta t_k)/2} + \frac{\beta}{l}\Theta_{k,0}^{*} + \frac{\beta\lambda}{l} \sum_{m=1}^{2} c_{k,m}^{(j)} \Theta_{k,m}^{*}, \\ C_k^{**(j+1)} &= C_k^- e^{-\lambda\Delta t_k} + \frac{\beta}{l}(\Theta_{k,0}^{*} + \Theta_{k,0}^{**}) + \frac{\beta\lambda}{l} \sum_{m=1}^{2} c_{k,m}^{(j)} (\Theta_{k,m}^{*} + \Theta_{k,m}^{**}). \end{aligned} \tag{30}$$

If we draw again the parabola (19), the change $j \to (j+1)$ having already been made, through the points C_k^- (the fit here is automatic), $C_k^{*(j+1)}$, $C_k^{**(j+1)}$, after recognizing that equations (30) are going to constitute an algebraic system of linearly independent equations for the two unknowns $c_{k,i}^{(j+1)}$, we still meet formulas similar to (21 a,b), in which the meaning for the b's is to be derived from (30)'s themselves. We thus write

$$\begin{aligned} c_{k,1}^{(j+1)} &= \frac{2b_{k,1}^{(j+1)} - b_{k,2}^{(j+1)}}{\Delta t_k} = \frac{4\left(C_k^{*(j+1)} - C_k^-\right) - \left(C_k^{**(j+1)} - C_k^-\right)}{\Delta t_k}, \\ c_{k,2}^{(j+1)} &= \frac{2\left(b_{k,2}^{(j+1)} - b_{k,1}^{(j+1)}\right)}{(\Delta t_k)^2} = 2\frac{\left(C_k^{**(j+1)} - C_k^-\right) - 2\left(C_k^{*(j+1)} - C_k^-\right)}{(\Delta t_k)^2}. \end{aligned} \tag{31}$$

Due to the linear dependence of the right hand sides of (31) on $c_{k,h}^{(j)}$ according to

$$\begin{aligned} C_k^{*(j+1)} - C_k^- &= \xi_1 + \sum_{m=1}^{2} \zeta_{1m} c_{k,m}^{(j)}, \\ C_k^{**(j+1)} - C_k^- &= \xi_2 + \sum_{m=1}^{2} \zeta_{2m} c_{k,m}^{(j)} \end{aligned} \tag{32}$$

where the following set of six definitions has been introduced:

$$\begin{aligned} \xi_1 &= -C_k^- \left(1 - e^{-\lambda(\Delta t_k)/2}\right) + \frac{\beta}{l}\Theta_{k,0}^*, \\ \xi_2 &= -C_k^- \left(1 - e^{-\lambda \Delta t_k}\right) + \frac{\beta}{l}(\Theta_{k,0}^* + \Theta_{k,0}^{**}), \end{aligned} \tag{33a}$$

$$\begin{aligned} \zeta_{1m} &= \frac{\beta\lambda}{l}\Theta_{k,m}^*, \\ \zeta_{2m} &= \frac{\beta\lambda}{l}(\Theta_{k,m}^* + \Theta_{k,m}^{**}), \qquad m = 1, 2. \end{aligned} \tag{33b}$$

We finally end up with the following expressions for the $(j+1)^{\text{th}}$ estimate of the parabola coefficients, that relate them *linearly* to their previous estimate:

$$\begin{aligned} c_{k,1}^{(j+1)} &= \frac{4\zeta_{11} - \zeta_{21}}{\Delta t_k} c_{k,1}^{(j)} + \frac{4\zeta_{12} - \zeta_{22}}{\Delta t_k} c_{k,2}^{(j)} + \frac{4\xi_1 - \xi_2}{\Delta t_k}, \\ c_{k,2}^{(j+1)} &= 2\frac{\zeta_{21} - 2\zeta_{11}}{(\Delta t_k)^2} c_{k,1}^{(j)} + 2\frac{\zeta_{22} - 2\zeta_{12}}{(\Delta t_k)^2} c_{k,2}^{(j)} + 2\frac{\xi_2 - 2\xi_1}{(\Delta t_k)^2}. \end{aligned} \tag{34}$$

An alternative presentation of the above result can help in simplifying the further steps. Let us define first the ket vectors

$$|K_k^{(j)}\rangle = \left| \begin{matrix} c_{k,1}^{(j)} \\ c_{k,2}^{(j)} \end{matrix} \right\rangle, \qquad j \in \mathbb{N}, \tag{35}$$

and

$$|b_k\rangle = \left| \begin{matrix} \dfrac{4\xi_1 - \xi_2}{\Delta t_k} \\ \dfrac{2\xi_2 - 4\xi_1}{(\Delta t_k)^2} \end{matrix} \right\rangle. \tag{36}$$

Equation 34 can thus be given the recursive form

$$|K_k^{(j+1)}\rangle = A_k |K_k^{(j)}\rangle + |b_k\rangle, \tag{37}$$

where the coefficient's matrix A_k happens to be independent of the iteration index j

$$A_k \doteq \begin{pmatrix} \dfrac{4\zeta_{11}-\zeta_{21}}{\Delta t_k} & \dfrac{4\zeta_{12}-\zeta_{22}}{\Delta t_k} \\ \dfrac{2\zeta_{21}-4\zeta_{11}}{(\Delta t_k)^2} & \dfrac{2\zeta_{22}-4\zeta_{12}}{(\Delta t_k)^2} \end{pmatrix} \doteq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}. \tag{38}$$

The iterative process for determining the coefficient of the parabola takes then the form

$$\begin{aligned} |K_k^{(0)}\rangle &= |0\rangle, \\ |K_k^{(1)}\rangle &= |b_k\rangle, \\ |K_k^{(2)}\rangle &= A_k|b_k\rangle + |b_k\rangle, \\ |K_k^{(3)}\rangle &= A_k(A_k|b_k\rangle + |b_k\rangle) + |b_k\rangle = A_k^2|b_k\rangle + A_k|b_k\rangle + |b_k\rangle, \\ &\cdots \\ |K_k^{(j+1)}\rangle &= \left(\sum_{n=0}^{j} A_k^n\right)|b_k\rangle. \end{aligned} \tag{39}$$

And, furthermore, provided that the limit process ($j \to \infty$) can be justified, the "best estimate" of the parabola coefficients would be

$$\boxed{|K_k^{\infty}\rangle = \lim_{j\to+\infty} |K_k^{(j)}\rangle.} \tag{40}$$

This result, of course, involves the convergence of the matrix power series $\sum_{n=0}^{\infty} A_k^n$, that implies, in its turn, for A_k that its spectral radius R_k satisfies the well-known condition $R_k < 1$. It has been verified at first that R_k happens to be monotonically decreasing as when Δt_k decreases. Furthermore, a theorem has been stated, concerning the asymptotic behavior of R_k as $\Delta t_k \to 0$. The full proof of it is reported in the next paragraph. We only anticipate here the result $R_k = O((\Delta t_k)^2)$, $(\Delta t_k \to 0)$. This statement justifies the limit process (40), with the only restriction that, would the interval I_k be too large, thus leading to a spectral radius $R_k > 1$, then we should be compelled to partition I_k itself, into two or more subintervals $I_{k_1}, I_{k_2} \ldots I_{k_N}$, for each one of which the condition $R_{k_i} < 1$ applies. As this has been proved to be always possible, we can thus forget about the problem of the spectral radius of A and simply refer to the case $R_k < 1$.

To make explicit the evaluation of the limit (40), without requiring any further numerical integration, we shall adopt the following procedure.

We determine first the eigenkets $|u_i\rangle$ of A_k by solving preliminarily the eigenvalue problem, the k index being partially dropped for simplicity,

$$A_k\,|u_i\rangle = \gamma_i\,|u_i\rangle, \qquad i = 1, 2, \tag{41}$$

where

$$|u_i\rangle \doteq \begin{vmatrix} u_i^{(1)} \\ u_i^{(2)} \end{vmatrix}\rangle$$

and then adjoint one, for the eigenbras $\langle v_l| \doteq \langle v_l^{(1)} v_l^{(2)}|$, after remarking, from (38), that all $a_{ik} \in \mathbb{R}$

$$\langle v_l|\,A_k = \gamma_l^{+}\,\langle v_l|, \qquad l = 1, 2. \tag{41'}$$

Obviously, the following relationship between direct γ_i and adjoint γ_l^{+} eigenvalues holds:

$$\gamma_l^{+} = \gamma_l^{*}, \qquad l = 1, 2, \tag{42}$$

where γ_l^{*} means the complex conjugate of γ_l.

Notice that, even for real A_k, one cannot exclude the occurrence of complex eigenvalues. In any case, however, both (41) and (41′) possess two linearly independent eigenvectors thus creating a *complete biorthogonal basis* in the two dimensional space of the real matrix A_k.

After a suitable normalization procedure, we can write down the following orthogonality and completeness relationships:

$$\langle v_i | u_k \rangle = \delta_{ik}, \tag{43a}$$

$$\sum_{i=1}^{2} |u_i\rangle\langle v_i| = I_{2x2}. \tag{43b}$$

In order to evaluate explicitly $|K_k^{\infty}\rangle$ having defined the projections of $|b_k\rangle$ along the bras $\langle v_j|$ by means of

$$b_{jk} \doteq \langle v_j | b_k \rangle, \tag{44}$$

we can thus write

$$\begin{aligned} |K_k^{(\infty)}\rangle &= \sum_{n=0}^{\infty} A^n \, |b_k\rangle = \sum_{n=0}^{\infty} A^n \left(\sum_{i=1}^{2} |u_i\rangle \, \langle v_i| \right) |b_k\rangle \\ &= \sum_{n=0}^{\infty} A^n \left[\sum_{i=1}^{2} |u_i\rangle \, b_{ik} \right] = \sum_{n=0}^{\infty} [\gamma_1^n \cdot b_{1k} \, |u_1\rangle + \gamma_2^n \cdot b_{2k} \, |u_2\rangle \,] \\ &= \frac{1}{1-\gamma_1} b_{1k} \, |u_1\rangle + \frac{1}{1-\gamma_2} b_{2k} \, |u_2\rangle \doteq \left| \begin{matrix} c_{k,1}^{(\infty)} \\ c_{k,2}^{(\infty)} \end{matrix} \right\rangle . \end{aligned} \tag{45}$$

Once $|K_k^{\infty}\rangle$ has been determined, we can go back to (25), in order to deduce, for $t \in I_k$

$$\boxed{P_k(t) \doteq \lim_{j \to \infty} P_k^{(j)}(t) \doteq P_k^{(\infty)}(t) = P_k^{(1)}(t) + \lambda \sum_{m=1}^{2} c_{k,m}^{(\infty)} \cdot T_{k,m}(t).} \tag{46}$$

This is just the transient power we were looking for. It fulfills both the differential system (2) and the initial conditions, consistently with the best parabolic representation of the smooth function $C(t)$. To follow the complete transient, we can now pass to the time interval $(k+1)$, after adjusting the initial conditions according to the results of the calculations just completed.

3. ON THE CONVERGENCE OF THE PARABOLIC APPROXIMATION PROCESS

Referring to the interval I_k, and to the definition (41) for the eigenvalues of the matrix A_k, expressed by means of (38), we recall that

$$R_k \stackrel{\text{def}}{=} \max_{i=1,2}(|\gamma_i|). \tag{47}$$

If the eigenvalues of A_k happen to be either complex conjugate to each other or real and coincident, we can simply write

$$|\gamma_1|^2 = |\gamma_2|^2 = a_{11}a_{22} - a_{12}a_{21}. \tag{48}$$

For the general case of real, distinct eigenvalues, we find

$$\gamma_1 = \frac{a_{11} + a_{22} - \sqrt{(a_{11} + a_{22})^2 - 4(a_{11}a_{22} - a_{12}a_{21})}}{2}, \tag{49a}$$

$$\gamma_2 = \frac{a_{11} + a_{22} + \sqrt{(a_{11} + a_{22})^2 - 4(a_{11}a_{22} - a_{12}a_{21})}}{2}. \tag{49b}$$

Going back to the previous definitions of the matrix elements a_{ik}'s, after a little algebra one can state that

$$a_{11}a_{22} - a_{12}a_{21} = \frac{4}{(\Delta t_k)^3}\left(\frac{\beta\lambda}{l}\right)^2 e^{-\lambda(t_k+(\Delta t_k)/2)}e^{-\lambda t_{k+1}} \cdot \left(\int_{t_k}^{t_k+(\Delta t_k)/2} T_{k1}(t')e^{\lambda t'}\,dt' \cdot \int_{t_k+(\Delta t_k)/2}^{t_{k+1}} T_{k2}(t')e^{\lambda t'}\,dt' - \int_{t_k}^{t_k+(\Delta t_k)/2} T_{k2}(t')e^{\lambda t'}\,dt' \cdot \int_{t_k+(\Delta t_k)/2}^{t_{k+1}} T_{k1}(t')e^{\lambda t'}\,dt'\right). \tag{50}$$

To each one of the four integrals in the above formula, the first mean value theorem of the integral calculus (see [8, p. 67]) applies, with the following result:

$$a_{11}a_{22} - a_{12}a_{21} = \frac{1}{(\Delta t_k)}\left(\frac{\beta\lambda}{l}\right)^2 \left(\frac{1-e^{-\lambda(\Delta t_k)/2}}{\lambda(\Delta t_k/2)}\right)^2 \cdot [T_{k1}(t_{k,(1)}) \cdot T_{k2}(t_{k,(3)}) - T_{k2}(t_{k,(2)}) \cdot T_{k1}(t_{k,(4)})], \tag{51}$$

where $t_{k,(1)}, t_{k,(2)} \in [t_k, t_k + (\Delta t_k)/2]$ and $t_{k,(3)}, t_{k,(4)} \in [t_k + (\Delta t_k)/2, t_{k+1}]$. Let us remind now that the exponential $e^{\Gamma_k(t)-\Gamma_k(t')}$, entering as a factor the integrands of $T_{km}(t)$ (see (26)) is a steadily increasing function of $t' < t$, for fixed t, in each subinterval of I_k, provided that $\Delta t_k < (\beta - \rho(t_k))/\alpha_k$. As a consequence, then

$$\sup_{t'\in[t_k,t]} e^{\Gamma_k(t)-\Gamma_k(t')} = 1, \qquad t \in [t_k, t_{k+1}], \quad \Delta t_k < \frac{\beta - \rho(t_k)}{\alpha_k}. \tag{52}$$

From the above equation and the previous definitions of the T_{km}'s integrals, it follows that the inequality

$$|T_{k1}(t_{k,(1)}) \cdot T_{k2}(t_{k,(3)}) - T_{k2}(t_{k,(2)}) \cdot T_{k1}(t_{k,(4)})| \leq c \cdot (\Delta t_k)^5, \qquad c = \text{const} \tag{53}$$

is satisfied and hence,

$$|a_{11}a_{22} - a_{12}a_{21}| \leq c \cdot \left(\frac{1-e^{-\lambda(\Delta t_k)/2}}{-\lambda(\Delta t_k)/2}\right)^2 \cdot (\Delta t_k)^4. \tag{54}$$

By a quite similar procedure, one can also deduce

$$|a_{11} + a_{22}| \leq c_k \cdot (\Delta t_k)^2 \left|\frac{1-e^{-\lambda(\Delta t_k)/2}}{-\lambda(\Delta t_k)/2}\right|, \qquad c_k = \text{const}. \tag{55}$$

Thus, from (48), (49), (54) and (55) we get, for all possible cases,

$$|\gamma_i| = O\left((\Delta t_k)^2\right), \qquad \Delta t_k \to 0. \tag{56}$$

From this result, associated to the definition (47) comes out the rigorous proof to the following theorem.

THEOREM. *The spectral radius of the matrix A is, asymptotically, for* $\Delta t_k \to 0$, *of the order of* $(\Delta t_k)^2$

$$R_k = O\left((\Delta t_k)^2\right), \qquad \Delta t_k \to 0. \tag{57}$$

The convergence of the limit processes (40) and (46), assumed on a physical basis in the previous paragraph, is thus completely proved.

Let us remark explicitly that the above proof does actually involve, as expected, *all of the dynamic equations* of the problem. As a matter of fact, the so called "hybrid" procedure, as described in this work, is by no means equivalent to a truncated power series technique for approximating the unknown of a single equation, out of a differential system of them.

4. A FEW COMMENTS ON THE PHYSICO-MATHEMATICAL RELEVANCE OF THE RESULT

Let us point out briefly that the "intrinsic self-consistency" of the solution (46) comes out from its peculiar built in property, that can be expressed as follows. If one introduces $P_k(t)$, represented through the rightmost side of (46), into the integral equation (12b), then the resulting precursor concentration $C(t)$ is such that its parabolic interpolation cannot be improved anymore by further adjustments of the parabola's coefficients, to be achieved through the requirement of a more and more accurate fulfillment of equation (12a).

As it was already anticipated, formula (46) is thus going to represent the "best solution" that one can provide to the differential system (2), while operating inside a subspace of the general solution vectors $|X(t)\rangle$, in which the second component is restricted to be a second order polynomial of t. The use of such a subspace, as pointed out in paragraph 1, can be easily justified on the physical ground, because of the quite slow variation of $C(t)$ over rather large integration intervals I_k, and even under the worse accident conditions. As a matter of fact, even in presence of "reactivity accidents," leading to explosive situations, in which $P(t)$ can undergo very rapid excursions, that could not be accurately foreseen by means of any extrapolation technique, the variation of $C(t)$, which is related, so to say, *to the total energy previously released* by the reactor and *not to the actual value of power*, is going to increase rather slowly. As a consequence the perfectly adjusted parabolic representation for $C(t)$ turns out to be adequate. And so is for the power $P(t)$, rigorously consistent with the associated precursor concentration being estimated by the above technique. We remark that statements just reported are by no means in disagreement with the well-known result of linear dynamics, stating that, during the asymptotic ($t \to \infty$) portion of a linear transient both $P(t)$ and $C(t)$ are expected to evolve with *the same exponential trend.* As a matter of fact, for violent transients, the dynamics is going to become nonlinear well before reaching its theoretically foreseen, purely exponential behavior.

The *main advantage* of the above procedure consists of the possibility of using quite large integration intervals Δt_k, wherever the linear time dependence of the reactivity function $\rho(t)$ can be assumed to hold. On the opposite, the length of the time steps to be adopted in a process of finite difference numerical integration would be somehow determined by the shortest time constant, i.e., the modulus of the inverse of the largest time eigenvalue of the system. This leads sometime to steps of the order of small fractions of milliseconds. Thus, the possibility of using, as in the present approach, time intervals Δt_k of the order of many tens of seconds, can lead to considerable time saving when setting up, for instance, real time power forecasting procedures.

5. THE COMPUTATION

A problem in the numerical analysis of this work is the need of evaluating integrals where the integrand possesses are improperly referred to as "a singularity." The integrands of the integrals to be calculated, such as that of equation (16), i.e.,

$$\int_{t_k}^{t} e^{\Gamma_k(t)-\Gamma_k(t')}\,dt' \tag{58}$$

or those of equations (26),

$$\int_{t_k}^{t} (t'-t_k)^m e^{\Gamma_k(t)-\Gamma_k(t')}\,dt' \doteq T_{k,m}(t), \qquad m=1,2 \tag{59}$$

are analytic over the whole interval of integration, but, while taking almost zero values on a quite large fraction of the integration domain, they present a strong peak at one end point. In this case a suitable variable transformation may be applied to the improper integrals, in order to remove the singularity: then the application of some quadrature formula will give good results.

For this scope, a characteristic of the trapezoidal rule can be used leading to extraordinarily high accuracy, when applied to an integral whose integrand is analytic and vanishes at the end points together with all its derivatives. For this and other reasons connected to the asymptotic error, the DE-rule (double exponential formula) (see [9], and also [4], for a comparison of different numerical techniques in a quite similar calculation) seems to be the more convenient variable transformation.

Since the integrals (58) and (59) over a finite interval $[t_k, t]$ can be transformed into integrals over the interval $[0, 1]$ by a simple linear mapping, we assume that the given integral is

$$I = \int_0^1 f(t')\,dt'. \tag{60}$$

By using the DE-rule

$$t' = \phi(x) = \frac{1}{2}\left[\tanh\left(\frac{\pi}{2}\sinh x\right) + 1\right], \tag{61}$$

we get

$$I = \int_{-\infty}^{\infty} f(\phi(x))\phi'(x)\,dx, \tag{62}$$

and the new transformed integrand function shows a double exponential decrease near the end points of the transformed domain because

$$|\phi'(x)| \sim \exp(-c\exp|x|), \qquad x \to \infty. \tag{63}$$

The efficiency of the formulas obtained by variable transformation still depends significantly from the choose of the mapping function $\phi(x)$. In DE-rule $\phi(x)$ is a function such that $\phi'(x)$ vanishes together with all its derivatives at the end points, so the error of this formula is expected to decrease very fast as the step used in the trapezoidal rule h tends to zero.

After the transformation we can approximate integral I by

$$I_h = h\sum_{n=-\infty}^{\infty} f\left(\frac{1}{2}\left[\tanh\left(\frac{\pi}{2}\sinh(nh)\right) + 1\right]\right)\frac{\frac{\pi}{4}\cosh(nh)}{\cosh^2\left(\frac{\pi}{2}\sinh(nh)\right)}. \tag{64}$$

We should recall here from [9] that a quadrature formula obtained by variable transformation usually has two kinds of errors. The first one is the error introduced when the integral is approximated by the trapezoidal rule, which is called the discretization error. The second one is the error introduced when the summation of the trapezoidal rule is truncated at a certain lower limit and an upper limit N of n, which is called the trimming error. The asymptotic error of the DE-rule in terms of the number N of points used is $\exp(-cN/\log N)$, where c is some constant depending on the formula and also on the integrand. We note that the DE-rule is more efficient than other transformations because by this one it is possible to explore into the end point singularity as deep as one wants; in fact, the DE-rule has infinite number of points in the neighborhood of the end points.

6. SOME REMARKS ON THE PROGRAM

To test this theory, a Fortran procedure is implemented on a VAX 4000-200. To integrate the well-behaved functions, quadrature formulas of NAG Fortran Library has been used. It is better to give some remarks necessary when one uses the DE-rule.

First (see [9]), in the denominator of $\phi'(x)$ (i.e., in $\cosh^2((\frac{\pi}{2})\sinh(nh))$ overflows arise where n is large. If the maximum absolute floating point number of the computer system used is approximately 10^m, then infinite summation in I_h must be truncated for

$$|n| \sim \frac{1}{h}\log\left(\frac{2m}{\pi}\log 10\right) \tag{65}$$

(i.e., at $10^m \sim \cosh^2((\frac{\pi}{2})\sinh(nh))$.

The second problem is a cancellation of significant digits in the computation of the integrand. To this end it may be useful to put (see [9])

$$W_n = \phi'(nh) \tag{66}$$

and

$$X_n = \begin{cases} (t - t_k)(1 - \phi(nh)), & n = 0, 1, 2, \ldots, \\ -(t - t_k)\phi(nh), & n = -1, -2, \ldots, \end{cases} \tag{67}$$

where $t' = \phi(x) = (1/2)[\tanh((\frac{\pi}{2})\sinh) + 1]$ and write the function subprogram $F(X)$ for

$$f(t') = e^{\Gamma_k(t) - \Gamma_k(t')} \tag{68a}$$

or

$$f(t') = (t' - t_k)^m e^{\Gamma_k(t) - \Gamma_k(t')} \tag{68b}$$

as

$$F(X) = \begin{cases} f(t_k - X), & -\frac{1}{2}(t - t_k) \leq X < 0, \\ f(t - X), & 0 \leq X \leq \frac{1}{2}(t - t_k). \end{cases} \tag{69}$$

Then

$$I_h = h \sum_{n=-\infty}^{-1} W_n F(X_n) + h \sum_{n=0}^{+\infty} W_n F(X_n). \tag{70}$$

To make this program easy to be used, a special mask, where all the inputs are shown, has been implemented. These values can be changed interactively. A satisfactory performance of the technique synthesized in equation (46) has been found, although the extension of the theory to the whole set of equations (1), and also to the transients with the decreasing reactivity is still underway. Intervals Δt_k of several tens of seconds have usually been handled, because the spectral radius R_k of the matrix A_k (see (38)) has been found to be less than one.

7. CONCLUSION

A new procedure for a quick integration of the point kinetics equations for fission reactors has been set up by adopting an hybrid technique, that relies on an *exact analytic integration of the reactor power equation*, associated to an iterative procedure, leading to a self-consistent estimate of the *best parabolic interpolation* of the precursor concentrations.

The preliminary numerical experience has shown that the procedure seems to be adequate to handle time steps up to several tens of seconds, provided that, for each one of them, the anticipated best fit of the reactivity curve is about to be linear in time. The overall performance of the method has been quite effective in the case of a single family of precursor. The extension of the procedure to the more significant case of six precursor families is still underway, together with the comparative assessment of its competitiveness, as far as the calculation time and allowable extent of the power forecast interval are concerned, whenever a preassigned accuracy for the output estimate is to be met.

It is expected that this approach can be profitably used for an "*almost real time*" reactor power forecasting, even when the reactor is evolving toward unforeseen accident conditions. It can also be applied to the calculation of tridimensional power transients, whenever a suitable eigenfunctions expansion of the power can be easily provided.

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